

Exact expression for the number of states in lattice models

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We derive a closed-form exact combinatorial expression for the number of states in canonical systems with discrete energy levels. The expression results from the exact low-temperature power series expansion of the partition function. The approach provides interesting insights into basis of statistical mechanics. In particular, it is shown that in some cases the logarithm of the partition function may be considered the generating function for the number of internal states of energy clusters, which characterize system's microscopic configurations. Apart from elementary examples including the Poisson, geometric and negative binomial probability distributions for the energy, the framework is also validated against the one-dimensional Ising model.

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It has long been recognized that the number of states, $g(E)$, with a given value of the energy, E , is a key quantity in equilibrium statistical physics. In principle, all energy-related thermodynamic properties of a classical canonical system can be calculated once $g(E)$ is known. In particular, in the case of a system with discrete energy levels, the canonical partition function is $Z(\beta) = \sum_E g(E)e^{-\beta E}$, where the summation is over the allowed energy levels, and quantities such as the Helmholtz free energy, $F(\beta) = -\ln Z(\beta)/\beta$, the ensemble-averaged energy, $\langle E \rangle = -\partial \ln Z(\beta)/\partial \beta$, and the specific heat (which is related to energy fluctuations, $\langle E^2 \rangle - \langle E \rangle^2 = -\partial \langle E \rangle / \partial \beta$) can be simply obtained.

Due to the central role of the energy distribution function, a variety of theoretical and computational studies have addressed the problem of how to obtain $g(E)$, see e.g. [1–6]. On the other hand, relatively little was done to understand, how the state-space representation of a considered system relates to its energy distribution, and how to recover such an information from, for example, the partition function.

In this paper we derive a new and general combinatorial formula for the density of states. The formula results from the exact low-temperature power-series expansion of the canonical partition function. In our approach $g(E)$ is expressed by the so-called Bell polynomials, which have a very convenient combinatorial interpretation: they describe, how equal energy portions can cluster together within the studied system. This, in turn, gives insight into system's microscopic details.

In the low-temperature expansion of the partition function, $Z(\beta) = \sum_{\Omega} e^{-\beta E(\Omega)}$, microstates, Ω , are counted in order of their importance as the temperature is increased from zero [7, 8]. If the ground state of a system is known and if the successive excitations from this state can be classified in a simple way, one should, at least theoretically, be able to construct such a series, i.e.

$$Z(x) = \sum_{N=0}^{\infty} g(\varepsilon N) x^N, \quad (1)$$

where

$$x = e^{-\beta \varepsilon}, \quad (2)$$

and energy is considered to be discrete

$$E = \varepsilon N, \quad (3)$$

with ε representing a portion of energy and $N = 0, 1, 2, \dots$ (with the ground-state energy equal to zero).

In Eq. (1), $g(\varepsilon N)$ represents the number of microscopic configurations in which energy of the system is εN .

From Eq. (1) it is apparent that the exact distribution function for the energy, $g(\varepsilon N)$, can be determined from the coefficients of the partition function. As a rule, however, when the order of expansion is increased complexity of contributing terms also increases rapidly. In this context, a *rule of thumb* states that the work involved in *direct* calculating the next term, $g(\varepsilon N)$, is the same as that needed to calculate all the preceding terms, $g(0), g(\varepsilon), \dots, g(\varepsilon N - \varepsilon)$. For this reason, generation of lengthy low-temperature power-series for the partition function is thought to be a highly specialized art. That is why, even in the case of the two-dimensional Ising model on a square lattice, for which the method was primary advanced (see ch. 6 in [1], the exact distribution of energies was just obtained in 1996 [2, 9], nearly a half of a century after Kaufman's exact solution for the partition function [10]).

The aim of this paper is to show that the effort needed to calculate the coefficients of the low-temperature power-series expansion for the canonical partition function is greatly reduced by using the combinatorial scheme described below. The approach is very general and applies to any lattice model. We also argue that the framework provides interesting insights into basis of statistical mechanics. In particular, it is shown that in some cases the logarithm of the partition function, $\ln Z(x)$, may be considered the generating function for the number of internal states of energy clusters, which characterize system's microscopic configurations. Apart from elementary examples including the Poisson, geometric, and negative binomial probability distributions for the energy,

the framework is validated against the one-dimensional Ising model, which is not at all a trivial example since its ordering temperature is zero, and the series, Eq. (1), is known to diverge at $x = 0$ as expected for a model with a zero temperature phase transition [8].

Derivation of the main result. To derive the main result of this paper, which is the general combinatorial formula for the number of states, we begin with the well-known relation between the canonical partition function and the Helmholtz free energy, i.e.

$$Z(x) = e^{A(x)}, \quad (4)$$

where x is the expansion variable of the low-temperature series, Eq. (2), and

$$A(x) = \ln Z(x) = \sum_{n=0}^{\infty} a_n \frac{x^n}{n!} = -\beta F(\beta), \quad (5)$$

with $a_n = \partial^n A(x)/\partial x^n|_{x=0}$. Then, using the generating function for Bell polynomials, $Y_N(\{a_n\})$, which are the polynomials with a sequence of parameters $\{a_n\} = a_1, a_2, \dots, a_N$, given by the formal power series expansion [11], Eq. (4) can be written as

$$Z(x) = \exp \left[\sum_{n=0}^{\infty} a_n \frac{x^n}{n!} \right] = e^{a_0} \sum_{N=0}^{\infty} \frac{1}{N!} Y_N(\{a_n\}) x^N. \quad (6)$$

In the last formula, the complete Bell polynomials, $Y_N(\{a_n\})$, are defined as follows

$$Y_0(\{a_n\}) = 1, \quad (7)$$

and for all $N \geq 1$

$$Y_N(\{a_n\}) = \sum_{k=1}^N B_{N,k}(\{a_n\}), \quad (8)$$

where $B_{N,k}(\{a_n\})$ represent the so-called partial (or incomplete) Bell polynomials, which can be calculated from the expression below

$$B_{N,k}(\{a_n\}) = N! \sum_{n=1}^{N-k+1} \prod_{n=1}^{N-k+1} \frac{1}{c_n!} \left(\frac{a_n}{n!} \right)^{c_n}, \quad (9)$$

where the summation takes place over all integers $c_n \geq 0$, such that

$$\sum_{n=1}^{N-k+1} c_n = k \quad \text{and} \quad \sum_{n=1}^{N-k+1} n c_n = N. \quad (10)$$

Finally comparing Eqs. (1) and (6), one gets the exact expression for the number of states:

$$g(\varepsilon N) = \frac{e^{a_0}}{N!} Y_N(\{a_n\}). \quad (11)$$

The basic difficulty with Eq. (11) may arise from an unacquaintance with Bell polynomials as given by Eqs. (8)

and (9). For this reason, we follow by explaining their meaning.

Suppose that N distinguishable particles are partitioned into k non-empty and disjoint clusters of $n_i > 0$ elements each, where $\sum_{i=1}^k n_i = N$. There are exactly

$$\binom{N}{n_1, \dots, n_k} = N! \prod_{i=1}^k \frac{1}{n_i!} = N! \prod_{n=1}^{N-k+1} \left(\frac{1}{n!} \right)^{c_n} \quad (12)$$

of such partitions, where $c_n \geq 0$ stands for the number of clusters of size n , with the largest cluster size being equal to $N - k + 1$, and where Eqs. (10) are satisfied. Suppose further that in such a composition clusters of the same size are indistinguishable from one another, and each of c_n clusters of size n can be in any one of $a_n \geq 0$ internal states. Then the number of partitions becomes, cf. with Eq. (12),

$$N! \prod_{n=1}^{N-k+1} \frac{1}{c_n!} \left(\frac{a_n}{n!} \right)^{c_n}. \quad (13)$$

Summing Eq. (13) over all integers $c_n \geq 0$ specified by Eqs. (10), one gets the partial Bell polynomial, $B_{N,k}(\{a_n\})$, which is defined by Eq. (9). If for all $n \geq 1$ the coefficients $a_n \geq 0$, the polynomial describes the number of partitions of a set of size N with exactly k subsets, where each coefficient, a_n , represents the number of internal states of a cluster of size n . Finally, summing the partial polynomials over k one gets the complete Bell polynomial, $Y_N(\{a_n\})$, the combinatorial meaning of which is obvious.

According to the explanations above the main result of this paper, Eq. (11), shows how equal energy portions, ε , are distributed, and how they cluster together within the system whose structural details are hidden in the coefficients $\{a_n\}$. If the coefficients are non-negative, i.e. $\forall_{n \geq 1} a_n \geq 0$, they can be interpreted as thermodynamic probabilities of energy clusters of a given size. Otherwise, their meaning is not clear.

In what follows, the Poisson and the negative binomial distributions are discussed as elementary mathematical examples of application of the combinatorial approach. The advantages of the new framework with respect to traditional methods of statistical mechanics are enhanced with reference to the one-dimensional Ising model.

Poisson distribution. As the first example, the Poisson distribution for the energy of a canonical system is considered,

$$P(E) = \frac{e^{-\langle E \rangle} \langle E \rangle^E}{E!}, \quad (14)$$

where, see Eq. (3), $\varepsilon = 1$ and $E = N = 0, 1, 2, \dots$. In order to bring Eq. (14) into the canonical form,

$$P(E) = g(E) \frac{e^{-\beta E}}{Z(\beta)}, \quad (15)$$

one has to assume that $\langle E \rangle = e^{-\beta}$. Then, the Poisson distribution can be written as

$$P(E) = \frac{1}{E!} \frac{e^{-\beta E}}{e^{e^{-\beta}}}, \quad (16)$$

where (compare Eqs. (15) and (16))

$$g(E) = \frac{1}{E!} \quad \text{and} \quad \ln Z(\beta) = e^{-\beta}. \quad (17)$$

To verify the combinatorial approach introduced in this paper, let us first notice that in the case of the Poisson distribution $x = e^{-\beta}$, Eq. (3). Therefore, the logarithm of the partition function is simply, cf. Eqs. (5) and (17),

$$A(x) = x. \quad (18)$$

The identity function for $A(x)$ provides a very significant sequence of the coefficients $\{a_n\}$ for the energy distribution function, Eq. (11), i.e.

$$a_0 = 0 \quad \text{and} \quad \{a_n\} = 1, 0, 0, \dots, 0. \quad (19)$$

The sequence states that in the case of a canonical system with the Poisson distribution of energy, energy portions, $\varepsilon = 1$, are independent from each other. In some sense it means that such a system is structureless (it may, for example, consists of noninteracting parts).

Finally, inserting the obtained coefficients into Eq. (11) one can easily get the energy distribution function, Eq. (17),

$$g(N) = \frac{1}{N!} Y_N(1, 0, 0, \dots, 0) = \frac{1}{N!}, \quad (20)$$

where $Y_N(1, 0, 0, \dots, 0) = 1$, because there is only one composition of a set of size N in which only clusters of size $n = 1$ may exist ($a_1 = 1$ and $a_n = 0$ for all $n > 1$).

Negative binomial distribution. As the second example the negative binomial distribution for the energy of a canonical system is studied,

$$P(E) = \binom{E + r - 1}{E} (1 - x)^r x^E, \quad (21)$$

where $x \in (0, 1)$ and $r > 0$, while $\varepsilon = 1$ and $E = N = 0, 1, 2, \dots$, see Eq. (3). It is worth noting that among the discrete distributions, the negative binomial distribution, $NB(r, x)$, Eq. (21), is considered the discrete analogue of the Gamma distribution, $\Gamma(r, \beta)$, whose probability density function is $P(E) = \beta^r E^{r-1} e^{-\beta E} / \Gamma(r)$, where r is the so-called shape parameter. The analogy is even more apparent if one realizes that, in the case of $r = 1$ the negative binomial distribution becomes the geometric distribution, $NB(1, x)$, which is the discrete analogue of the exponential distribution, $\Gamma(1, \beta)$.

Bringing the negative binomial distribution, Eq. (21), into the canonical form, Eq. (15), for $x = e^{-\beta}$ one gets:

$$g(E) = \binom{E + r - 1}{E}, \quad (22)$$

and

$$A(x) = -r \ln(1 - x) = r \sum_{n=1}^{\infty} (n-1)! \frac{x^n}{n!}. \quad (23)$$

The series expansion of the logarithm of the partition function, $A(x)$, gives the following sequence of the coefficients $\{a_n\}$:

$$a_0 = 0 \quad \text{and} \quad \forall_{n \geq 1} a_n = r(n-1)!. \quad (24)$$

The sequence provides a meaningful microscopic information about the considered canonical system. First, it appears that the parameter r describes the degeneracy of internal states of the energy-clusters, and the lack of degeneracy, $r = 1$, results in the geometric/exponential distribution. Second, since $(n-1)!$ is the number of permutations of n objects where the first object is fixed, the only reasonable explanation behind $a_n \propto (n-1)!$ is the linear ordering of energy portions within the clusters. At first glance the idea of ordering of indistinguishable energy portions may seem unacceptable, but it gets intelligibility if one realizes that in some sense energy portions become distinguishable once they, for example, become interaction energies between given pairs of particles.

To validate the main result of this paper, Eq. (11), one has to insert the coefficients given by Eqs. (24) into the mentioned expression. After some algebra one gets Eq. (22):

$$g(N) = \frac{1}{N!} Y_N(\{r(n-1)!\}) \quad (25)$$

$$= \frac{1}{N!} \sum_{k=1}^N r^k B_{N,k}(0!, 1!, 2!, \dots) \quad (26)$$

$$= \frac{1}{N!} \sum_{k=1}^N r^k \binom{N}{k} = \binom{N+r-1}{N}, \quad (27)$$

where basic combinatorial identities have been used, including [11, 12]: i. the generating function for the unsigned Stirling numbers of the first kind, $\binom{N}{k}$, and ii. properties of Bell polynomials, i.e. $B_{N,k}(\{ru^k a_n\}) = r^k u^N B_{N,k}(\{a_n\})$ and $B_{N,k}(\{(n-1)!\}) = \binom{N}{k}$ [13].

One-dimensional Ising model. The Hamiltonian of the closed chain of V Ising spins, $\{s_i\}$, with nearest-neighbor interactions in the absence of external magnetic field can be written as

$$H(\{s_i\}) = -J \sum_{i=1}^V s_i s_{i+1}, \quad (28)$$

where $J > 0$, $s_i = \pm 1$, and the periodic boundary condition is imposed by assuming that $s_{V+1} = s_1$. In the thermodynamic limit, $V \gg 1$, the partition function of the model is given by

$$Z(\beta) = (e^{\beta J} + e^{-\beta J})^V. \quad (29)$$

To use Eq. (11) to calculate the number of states, $g(E)$, characterizing the model, one must first rescale its energy, E , because in the present form of the Hamiltonian, Eq. (28), the ground state energy is negative, $H(\{-1\}) = H(\{+1\}) = -JV$, whereas it should be at least equal to zero, see Eqs. (1), (3) and (2). The problem can be solved by adding to Eq. (28) a constant, JV , so that for all the spin configurations, $\{s_i\}$, the modified Hamniltonian,

$$H^*(\{s_i\}) = -J \sum_{i=1}^V s_i s_{i+1} + JV, \quad (30)$$

results in non-negative energy

$$E^* = E + JV \geq 0. \quad (31)$$

With this change, the partition function of the model becomes

$$Z^*(\beta) = e^{-\beta JV} Z(\beta) = (1 + e^{-2\beta J})^V, \quad (32)$$

but statistical properties of the chain of spins, $\{s_i\}$, remain the same, as compared with the original Ising model. In particular, the probability distributions for spin configurations, $P(\{s_i\}) = \exp[-\beta H(\{s_i\})]/Z(\beta)$ and $P^*(\{s_i\}) = \exp[-\beta H^*(\{s_i\})]/Z^*(\beta)$, coincide with one another. The same applies to probability distributions for the energy, $P(E) = g(E)e^{-\beta E}/Z(\beta)$ and $P^*(E^*) = g^*(E^*)e^{-\beta E^*}/Z^*(\beta)$.

In view of the above considerations one can see that

$$g(E) = g^*(E^*) = g^*(E + JV). \quad (33)$$

Thus, to determine the number of states for the one-dimensional Ising model, $g(E)$, one can calculate $g^*(E^*)$, and then change the variables E^* and E according to Eq. (31).

In the following, for simplicity one assumes in Eq. (32) that $J = 1/2$. Then, the logarithm of the partition function, $\ln Z^*(\beta)$ can be written as, Eq. (5),

$$A^*(x) = V \ln(1 + x) = V \sum_{n=1}^{\infty} (-1)^{n-1} (n-1)! \frac{x^n}{n!}, \quad (34)$$

where $\varepsilon = 1$ and $x = e^{-\beta}$. From the series expansion, it is obvious that the coefficients $\{a_n\}$, i.e.

$$a_0 = 0 \quad \text{and} \quad \forall_{n \geq 1} a_n = V(-1)^{n-1}(n-1)!, \quad (35)$$

do not satisfy the condition of non-negativity, which (if satisfied) allows to conclude on state space representation of the considered model. Nevertheless, the knowledge of $\{a_n\}$ (regardless of their sign) enables a direct validation of the combinatorial approach. By inserting the coefficients into the expression for the energy distribution function, Eq. (11), after some algebra one gets, for $N = E^*$,

$$g^*(N) = \frac{1}{N!} Y_N(\{V(-1)^{n-1}(n-1)!\}) \quad (36)$$

$$= \frac{1}{N!} \sum_{k=1}^N V^k (-1)^{N-k} \begin{bmatrix} N \\ k \end{bmatrix} = \binom{V}{N}, \quad (37)$$

where $(-1)^{N-k} \begin{bmatrix} N \\ k \end{bmatrix}$ is the signed Stirling number of the first kind. From the last expression one immediately gets

$$g(E) = \binom{V}{E + V/2}, \quad (38)$$

where E is the energy of the original Ising model described by Eqs. (28) and (29).

The obtained result, Eqs. (37) and (38), is exactly the expected one: the number of microscopic configurations of the closed chain of V Ising spins is equal to the number of ways to choose positions for E^* pairs of equal spins, $\{+1, +1\}$ and $\{-1, -1\}$, from the available V positions.

Summary. Our approach differs crucially from previous works on the number of states. We use the combinatorial mathematics of exponential generating functions to obtain the exact low-temperature power-series expansion of the canonical partition function. The expansion results in the exact expression for the energy distribution in arbitrary lattice models. Apart from elementary examples including the Poisson, geometric, and negative binomial probability distributions for the energy, the framework is validated against the one-dimensional Ising model. The work on the application of the formalism to the Ising model on a square lattice is in progress and will be reported in a future article to follow.

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